



# ***Selected Enhanced Fidelity AIM Methods***

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Mike Uchic, & Jeff Simmons***

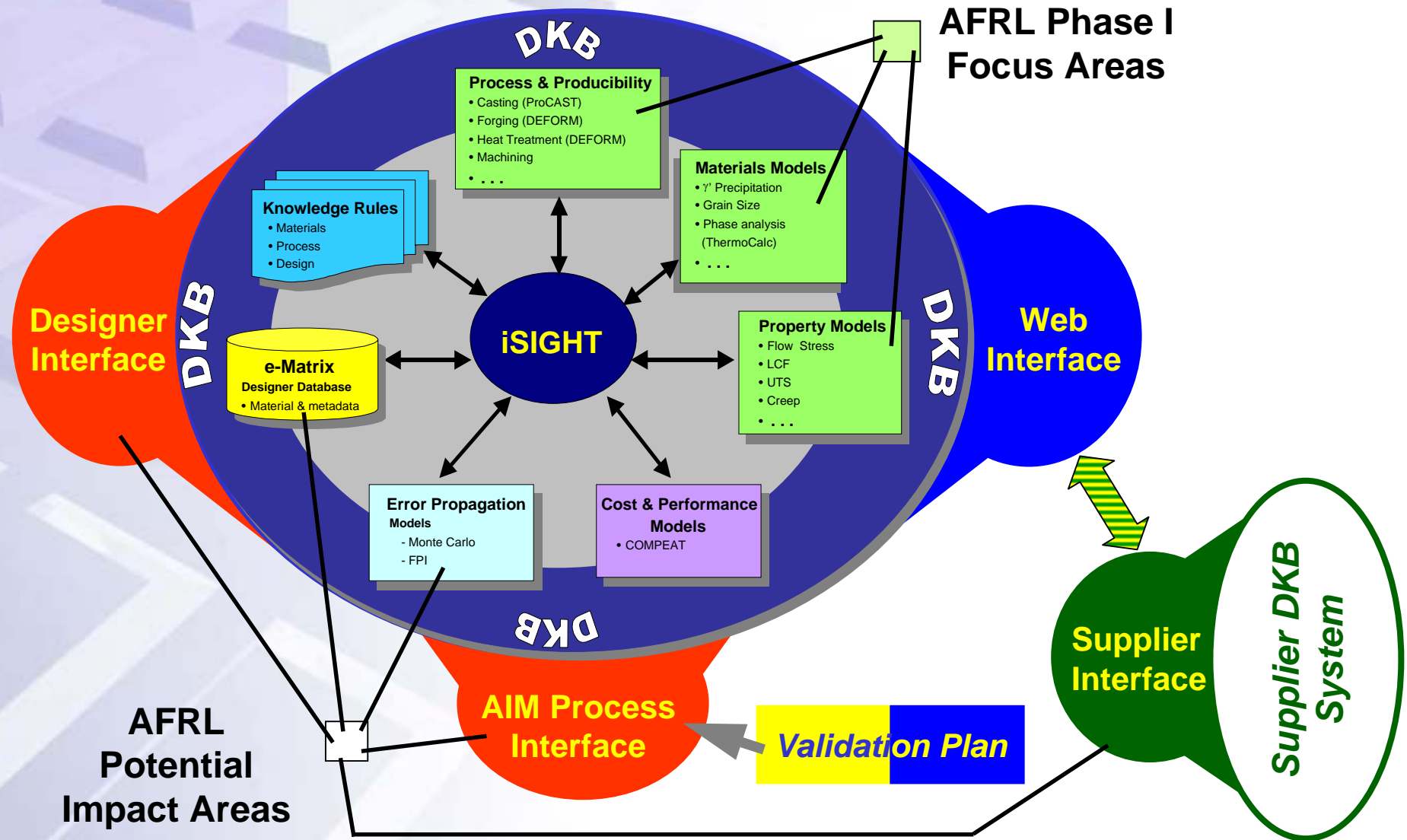
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# AIM System Architecture





## ***What About Phase II & Beyond?***

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**In general, demand is for methods to treat unknown (without database)**

**Numerical descriptions needed for scope & fidelity in performance prediction (property minima & fracture are locally dominated)**

**These require development and adaptation to system architecture**

**Thus AFRL Focus:**

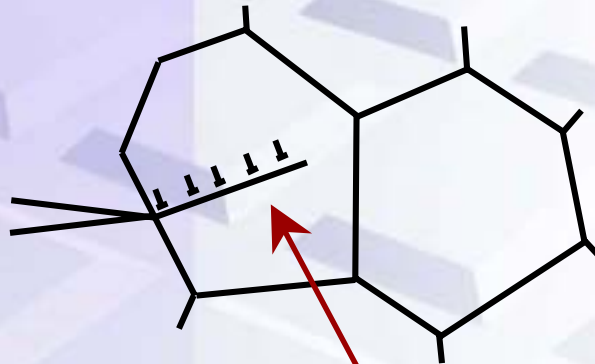
**Prediction, quantification & representations of structure evolution & kinetics**

**Structure-sensitive numeric descriptions of properties**

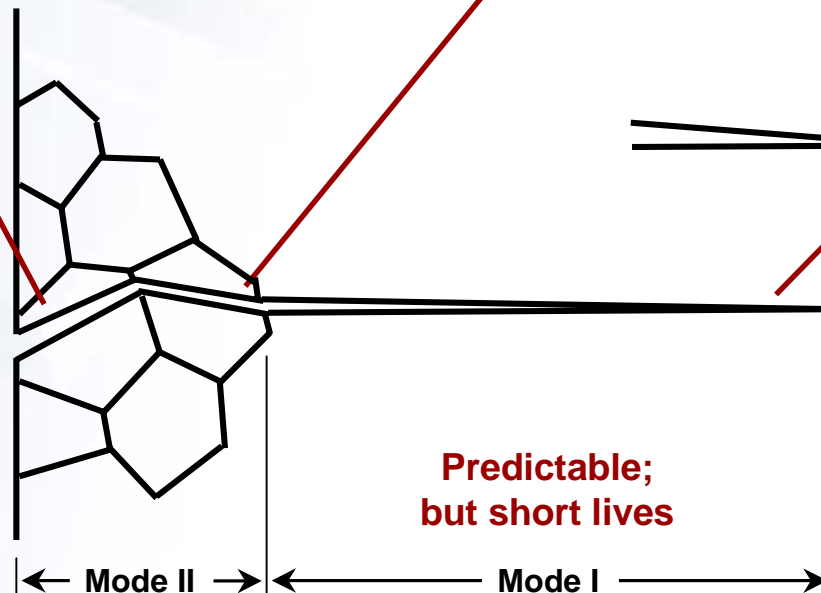
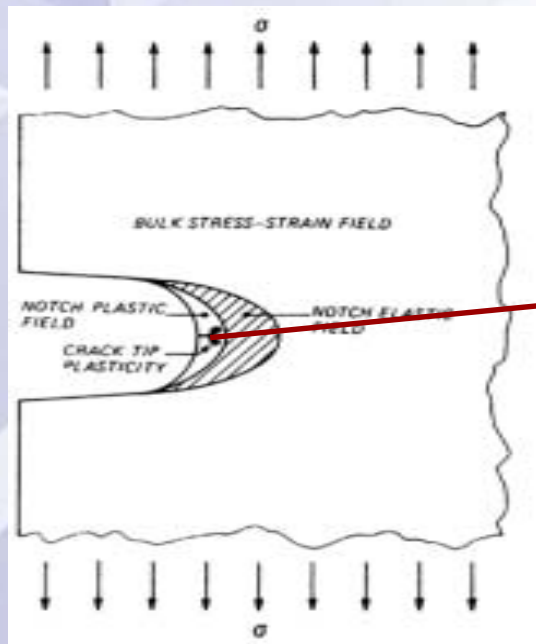
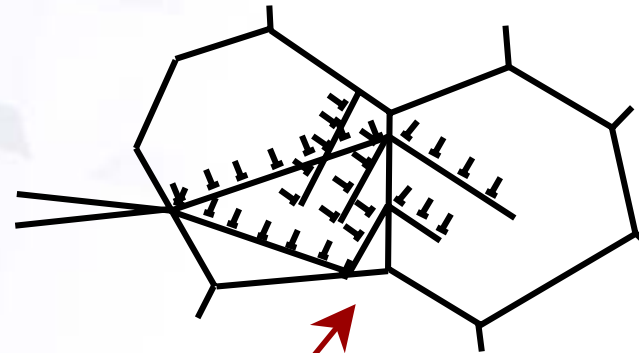
**Overlay of 'homogenized' or 'fast-acting' models, validation/tuning procedures, & interlace with design/architecture**

# Need for Microstructure-Based Plasticity

Short cracks & initiation;  
slip & environment

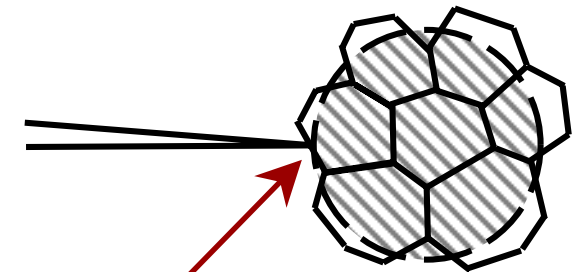


'Longer' cracks;  
microstructure &  
*local* plasticity  
dominated



Most of life;  
unpredictable

Predictable;  
but short lives



Long cracks;  
linear elastic  
fracture  
mechanics

# From Concepts to Realities

## Briefings on Today's Progress

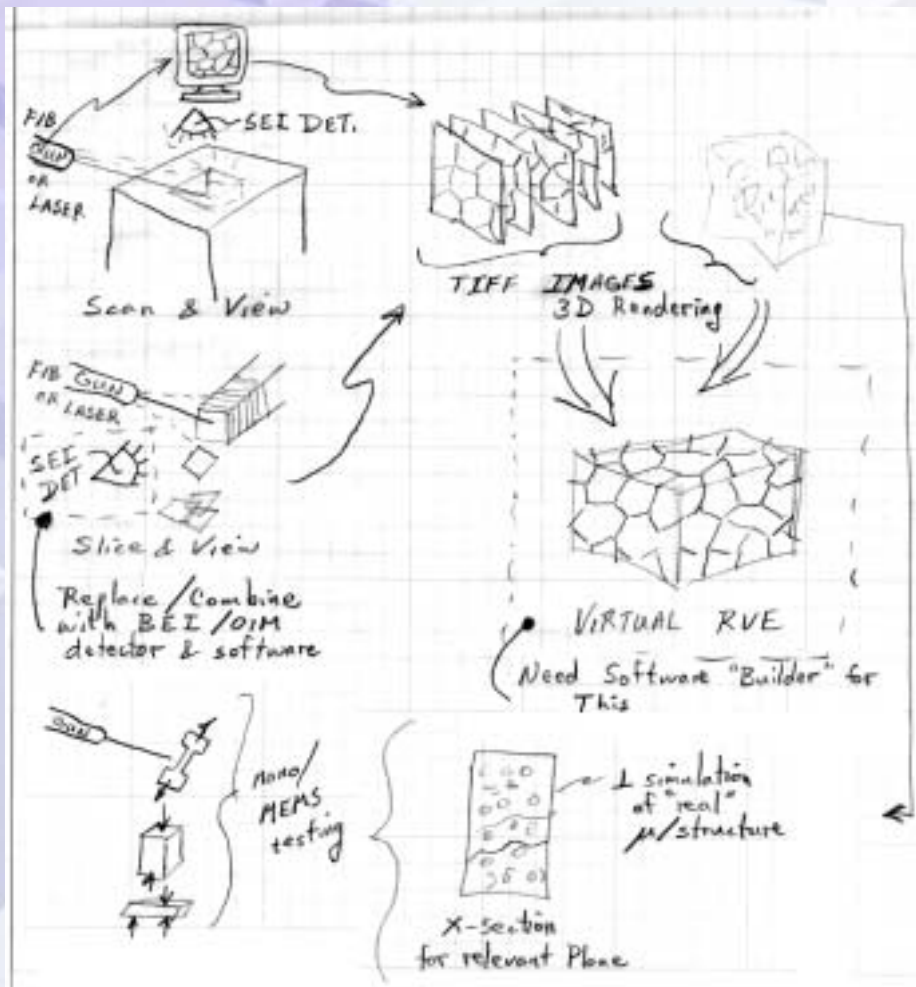
Phase Field (Simmons, 20min)

Plasticity Modeling (Parthasarathy, 20min)

Advanced Experimental Methods

- 3D Quantification (Uchic, 10min)
- Representation (Simmons, 15min)
- Micro- & Nano-scale Tests (Uchic, 15min)

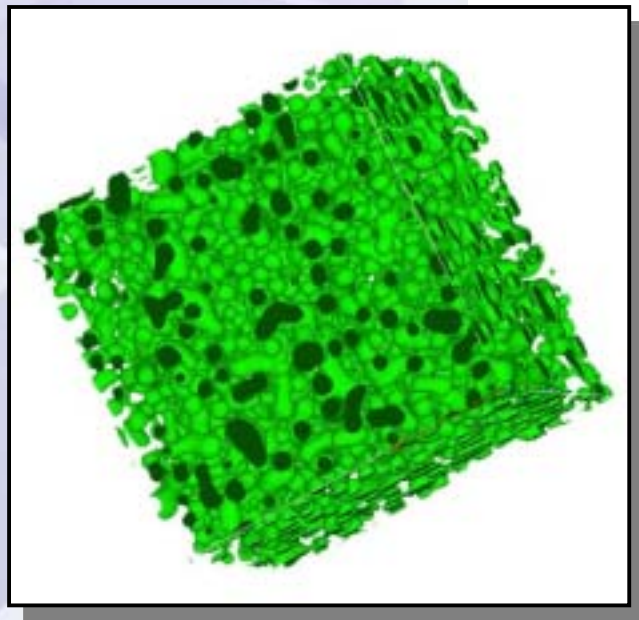
Broader View & Discussion  
(Dimiduk, All)



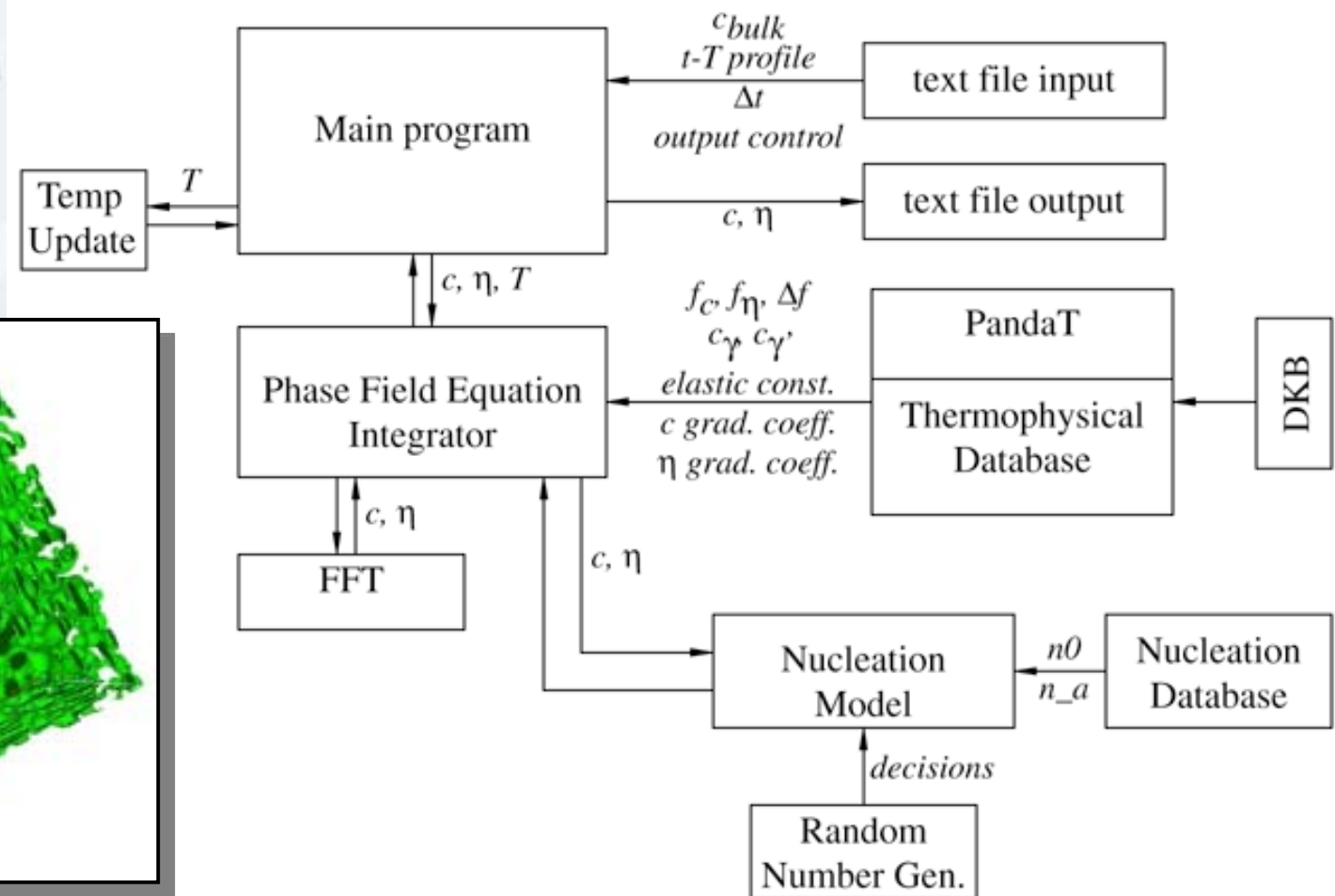
*Last year's 'sketchy' concept*



# Architecture & Implementation of Phase Field Software



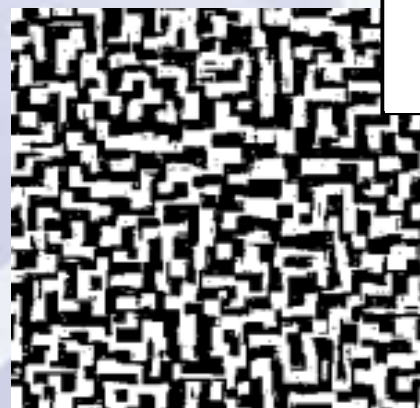
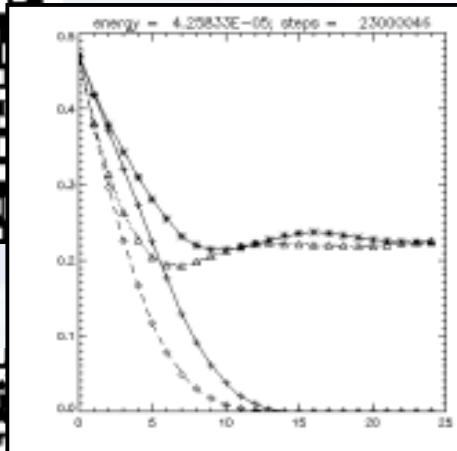
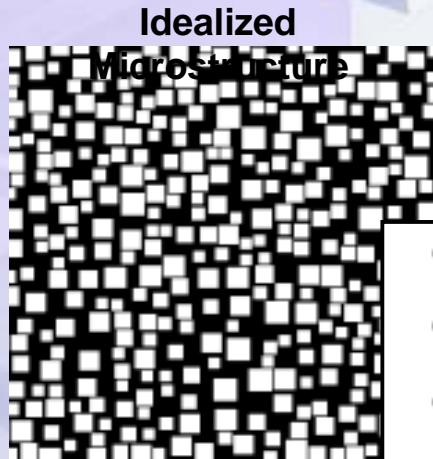
3D, Isothermal  $\gamma$ - $\gamma'$  Coarsening



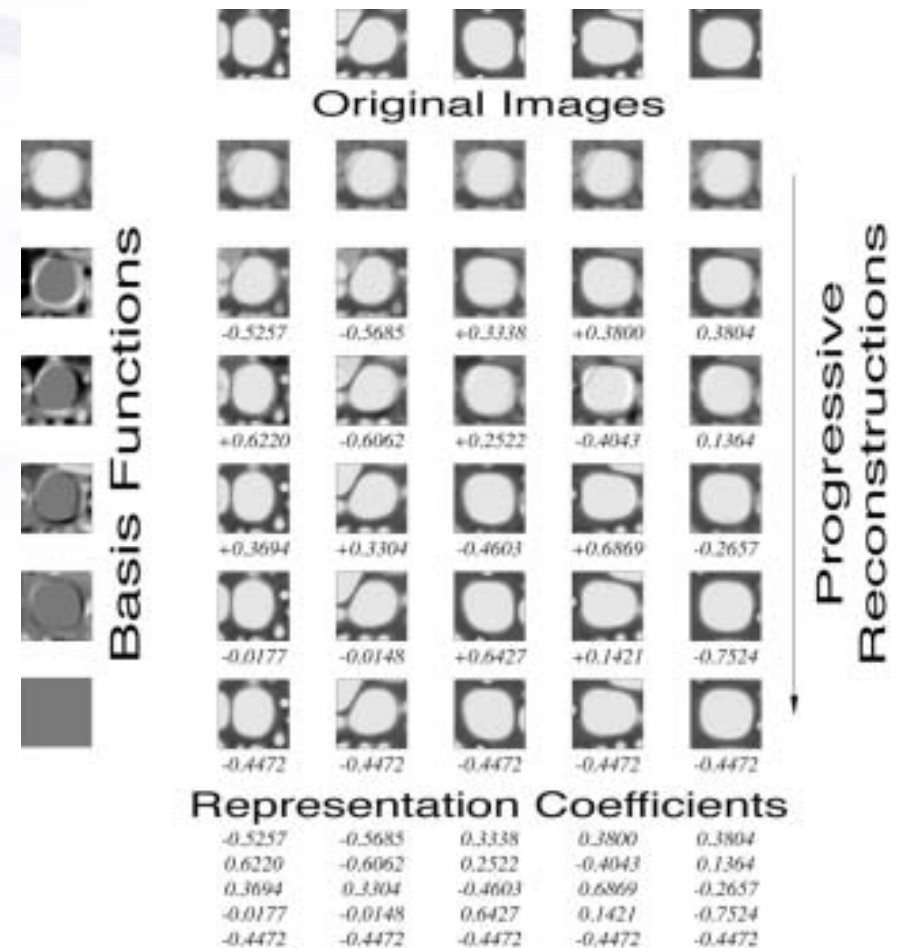
**Clear framework identified...real dimensionality, thermodynamics evolving!**

# Microstructure Representations

## 2-Point & Lineal Path Functions



Monte Carlo  
Reconstructed  
Representative  
Microstructure



## Principal Component Analysis (KLT)

Revolutionary longer-term approach to capture all information contained in microstructure

# Beyond Analytical Strength Models

## Needs Development Within Atomistics

$$\sigma_y(C_i, T, \varepsilon, \dot{\varepsilon}, \dots) = f_\gamma \left( \frac{T_o}{T} \right) \left( \sum_i \frac{dc}{\sqrt{dC_i}} \sqrt{C_i} \right) + M f_t \left( \frac{\Gamma_{APB}}{b} \right)$$

## Obtain by Dislocation Kinetics Simulation

$$+ \begin{cases} M \frac{4}{\pi^{1.5}} \cdot \frac{T_L}{bd_s} \sqrt{f(1-f_p)} \sqrt{\left( \frac{\pi d_s \Gamma_{APB}}{2T_L} - 1 \right)} & \text{strong coupling} \\ M \left[ \left( \frac{\Gamma_{APB}}{2b} \right)^{1.5} \sqrt{\frac{2bd_s f(1-f_p)}{T_L}} \cdot \frac{4}{\pi^{1.5}} - \frac{\Gamma_{APB} f(1-f_p)}{2b} \right] & \text{weak coupling} \end{cases}$$

see Reppich

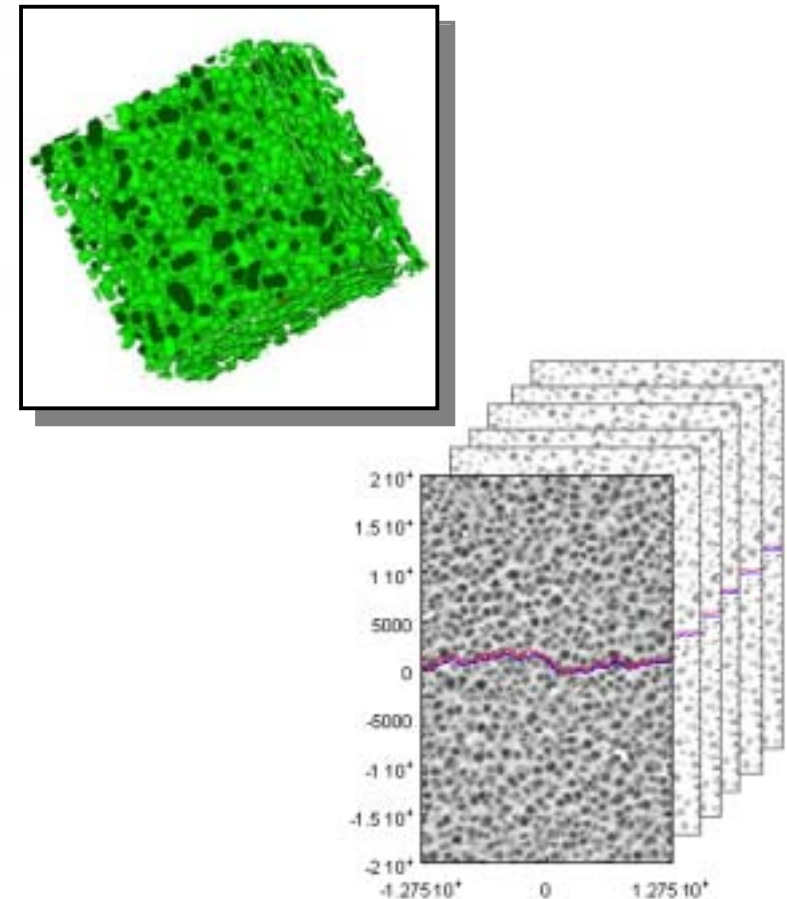
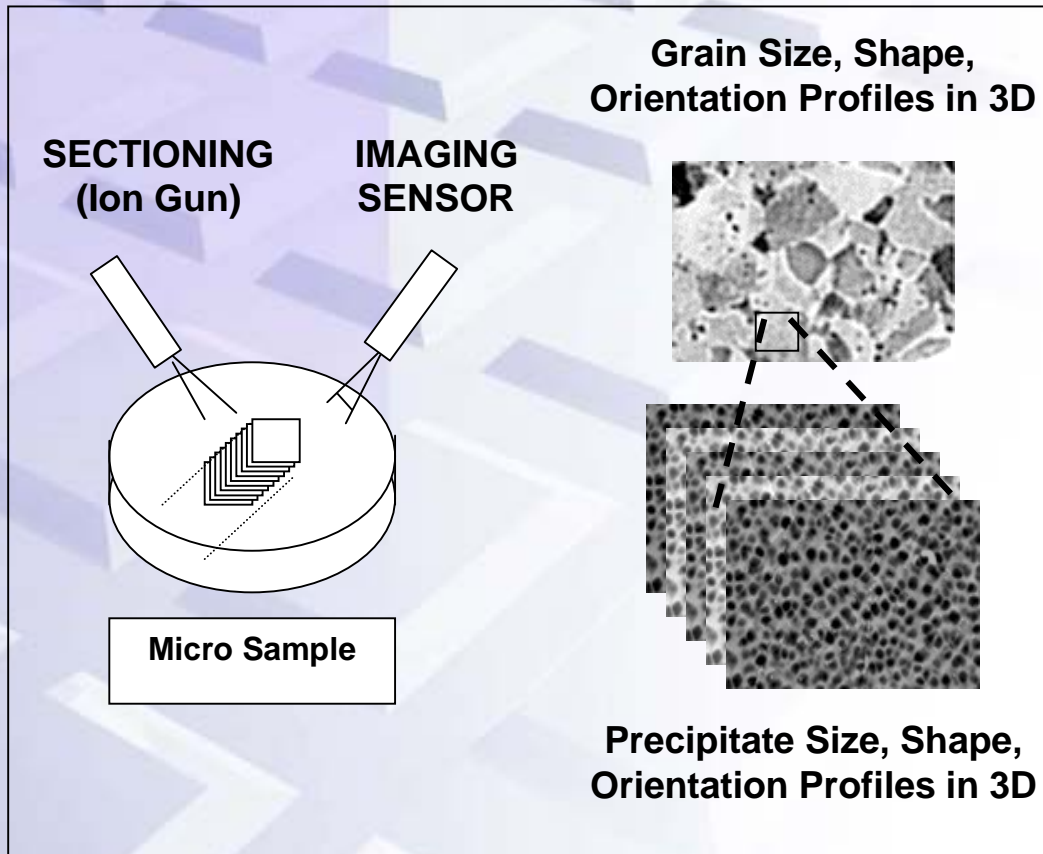
## Obtain by FEM Simulation of Grain Distribution Effects

$$+ f_p \left[ \sigma(T)_{Ni_3Al} + \sum_i \left( \frac{dc}{dC_i} C_i \right) \right] + f_p k_y^{\gamma'} \frac{1}{\sqrt{d_{\gamma'}}} + (1 - f_p) k_y^{\gamma} \frac{1}{\sqrt{d_{\gamma}}}$$

**Numeric methods need and interface to AIM system**



# Unknown New Materials



**3D sectioning experiments**

**Advanced simulation & experiments**

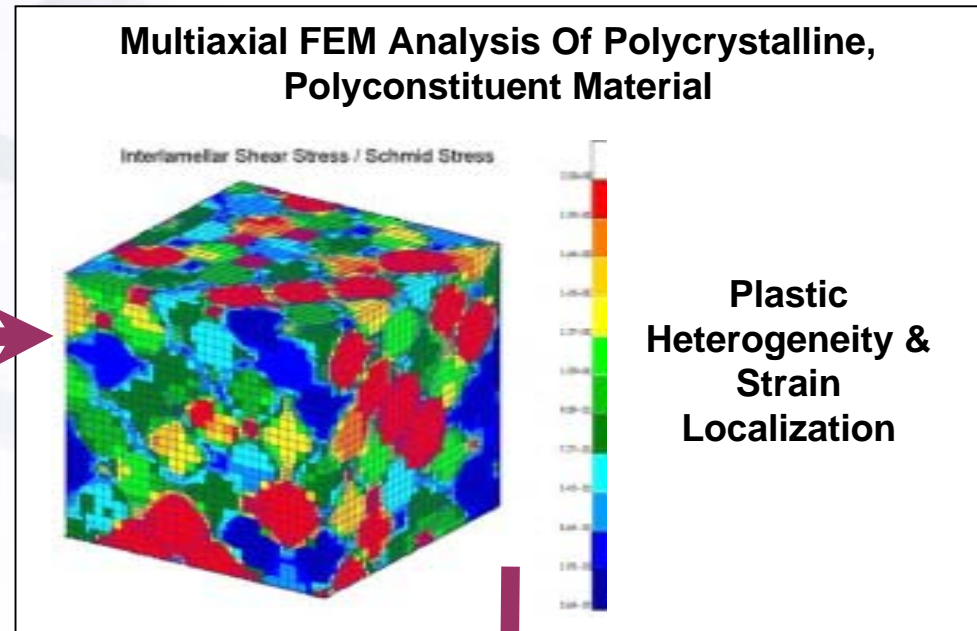
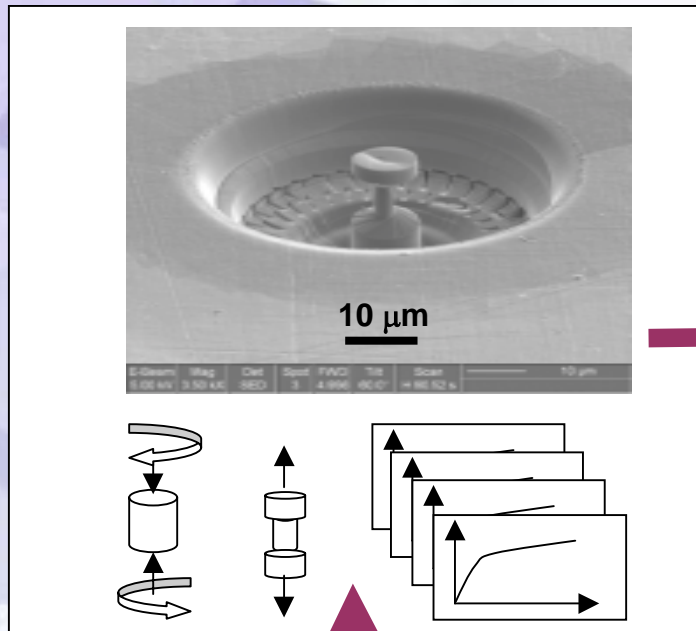
**Small-scale property measurements**

⇒ **3D virtual structure representations**

⇒ **intrinsic grain-level properties**

⇒ **model parameterization**

# Treating Unknown New Materials



**Properties of Representative Volume Element (RVE) From Mesoscale and Analytical Tools**

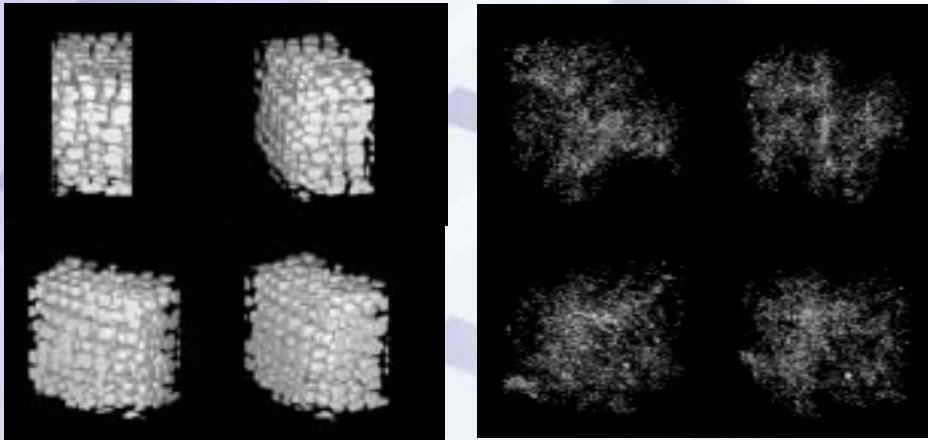
$$\dot{\tau} = \left\{ h - \left( \frac{\tau - \tau_o}{\tau_s - \tau_o} \right) h \right\} \left( \frac{\dot{\gamma}}{\dot{\gamma}_o} \right)^m$$

τ

γ

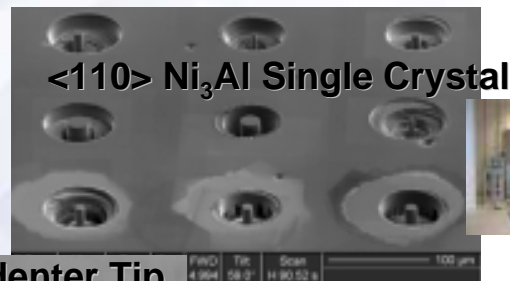
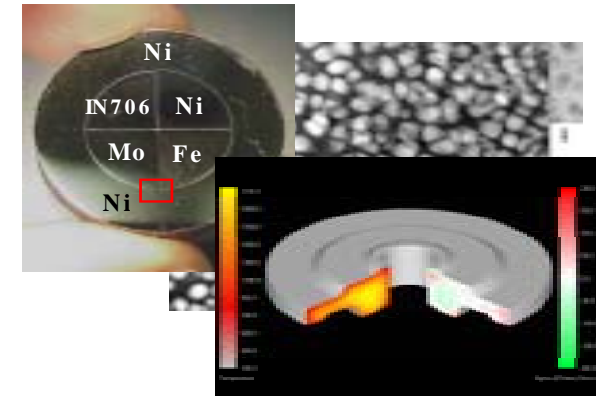
**Microstructure-Sensitive Representations (UMATs for 'intrinsic material' RVEs; results used in Ramberg-Osgood or Walker-like forms, or "Curve Generator," etc)**

# Efficient Experiments for New Materials

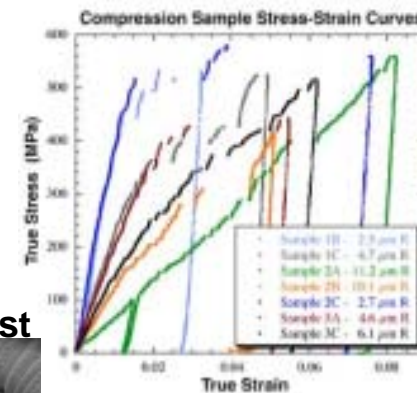
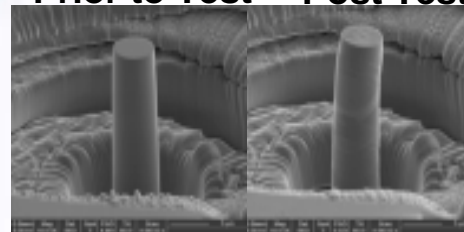


**3-Dimensional Characterization of  $\gamma'$  and Carbides**

## Rapid Experiments, Modeling, & Characterization



**Prior to Test Post Test**

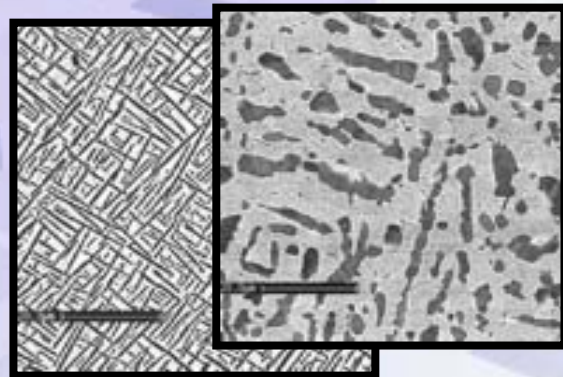


**Micro- & Nano-Scale Property Measurement**

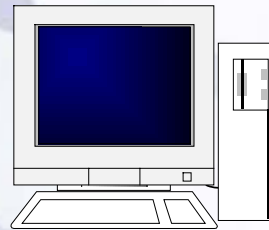
**Unprecedented Novel & Efficient Experiments Emerging!**



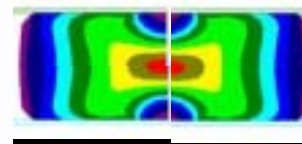
# Payoff: Materials & System Prognostics



Materials



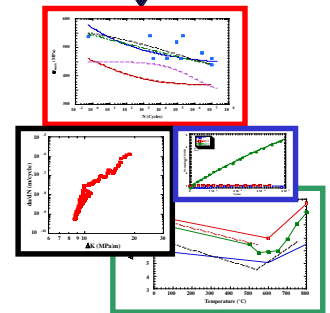
Mathematics



Experiment



Experience



Property Database

**Mathematics**

**State Awareness**

**Failure Physics**

**Data Fusion**

**Reasoning System**

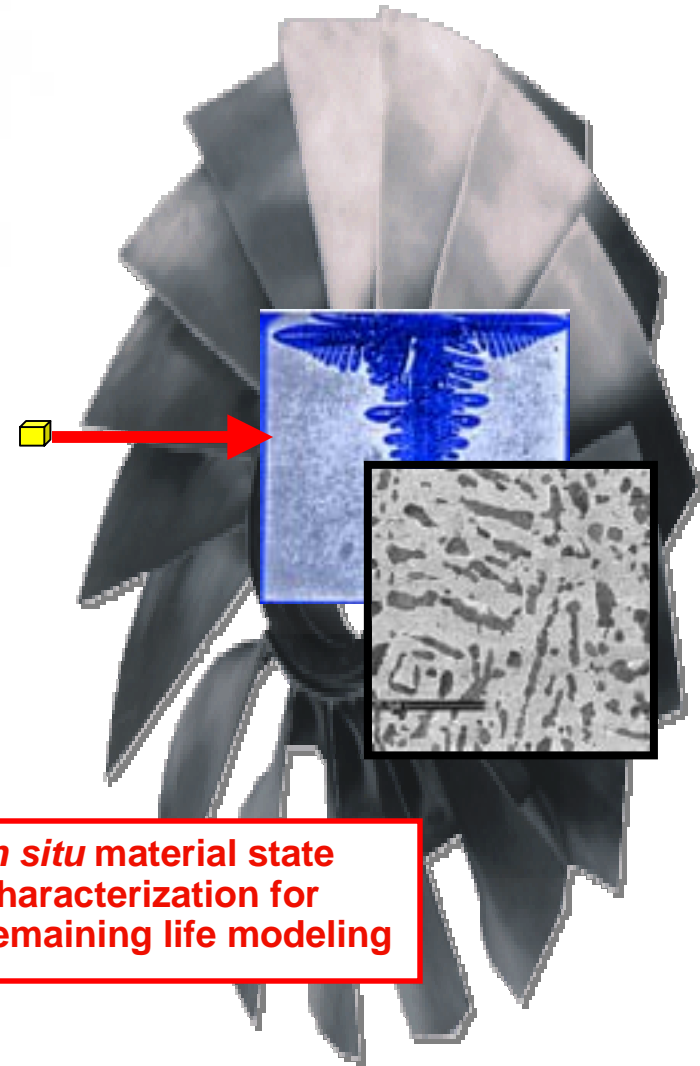


Combat System Readiness

**Prognostics**

## ***Material State Definition***

- Characterize each disk's microstructure and damage state at the mesoscale
- Utilize DARPA/AF AIM technology – stochastic life prediction
- Material state sensing
  - Electron backscatter diffraction (EBSD)
  - Acoustic attenuation
  - Others...
- Define the probability of cracking for each disk





## *MS & E Paradigm*

